PRISMS-PF: Precipitate Evolution

1 Variational formulation

The total free energy of the system (neglecting boundary terms) is of the form,

$$\Pi(c, \eta_1, \eta_2, \eta_3, \boldsymbol{\epsilon}) = \int_{\Omega} f(c, \eta_1, \eta_2, \eta_3, \boldsymbol{\epsilon}) \; dV \tag{1}$$

where c is the concentration of the β phase, η_p are the structural order parameters and $\boldsymbol{\varepsilon}$ is the small strain tensor. f, the free energy density is given by

$$f(c, \eta_1, \eta_2, \eta_3, \boldsymbol{\epsilon}) = f_{chem}(c, \eta_1, \eta_2, \eta_3) + f_{grad}(\eta_1, \eta_2, \eta_3) + f_{elastic}(c, \eta_1, \eta_2, \eta_3, \boldsymbol{\epsilon}) \tag{2}$$

where

$$f_{chem}(c, \eta_1, \eta_2, \eta_3) = f_{\alpha}(c) \left(1 - H(\eta_1) - H(\eta_2) - H(\eta_3)\right) + f_{\beta}(c) \left(H(\eta_1) + H(\eta_2) + H(\eta_3)\right)) + W f_{Landau}(\eta_1, \eta_2, \eta_3) \tag{3}$$

$$f_{grad}(\eta_1, \eta_2, \eta_3) = \frac{1}{2} \sum_{p=1}^{3} \boldsymbol{\kappa}_{ij}^{\eta_p} \eta_{p,i} \eta_{p,j} \tag{4}$$

$$f_{elastic}(c, \eta_1, \eta_2, \eta_3, \boldsymbol{\epsilon}) = \frac{1}{2} \boldsymbol{C}_{ijkl}(\eta_1, \eta_2, \eta_3) \left(\boldsymbol{\varepsilon}_{ij} - \boldsymbol{\varepsilon}^0_{ij}(c, \eta_1, \eta_2, \eta_3)\right) \left(\boldsymbol{\varepsilon}_{kl} - \boldsymbol{\varepsilon}^0_{kl}(c, \eta_1, \eta_2, \eta_3)\right) \tag{5}$$

$$\boldsymbol{\varepsilon}^0(c, \eta_1, \eta_2, \eta_3) = H(\eta_1)\boldsymbol{\varepsilon}^0_{\eta_1}(c) + H(\eta_2)\boldsymbol{\varepsilon}^0_{\eta_2}(c) + H(\eta_3)\boldsymbol{\varepsilon}^0_{\eta_3}(c) \tag{6}$$

$$\boldsymbol{C}(\eta_1, \eta_2, \eta_3) = H(\eta_1)\boldsymbol{C}_{\eta_1} + H(\eta_2)\boldsymbol{C}_{\eta_2} + H(\eta_3)\boldsymbol{C}_{\eta_3} + \left(1 - H(\eta_1) - H(\eta_2) - H(\eta_3)\right) \boldsymbol{C}_{\alpha} \tag{7}$$

Here $\boldsymbol{\varepsilon}^0_{\eta_p}$ are the composition dependent stress free strain transformation tensor corresponding to each structural order parameter.

2 Required inputs

- $f_{\alpha}(c), f_{\beta}(c)$ - Homogeneous chemical free energy of the components of the binary system, example form given in Appendix I
- $f_{Landau}(\eta_1, \eta_2, \eta_3)$ - Landau free energy term that controls the interfacial energy and prevents precipitates with different orientation varients from overlapping, example form given in Appendix I
- W - Barrier height for the Landau free energy term, used to control the thickness of the interface
- $H(\eta_p)$ - Interpolation function for connecting the α phase and the p^{th} orientation variant of the β phase, example form given in Appendix I
- $\boldsymbol{\kappa}^{\eta_p}$ - gradient penalty tensor for the p^{th} orientation variant of the β phase
- $\boldsymbol{C}_{\eta_p}$ - fourth order elasticity tensor (or its equivalent second order Voigt representation) for the p^{th} orientation variant of the β phase
- $\boldsymbol{C}_{\alpha}$ - fourth order elasticity tensor (or its equivalent second order Voigt representation) for the α phase
- $\boldsymbol{\varepsilon}^0_{\eta_p}$ - stress free strain transformation tensor for the p^{th} orientation variant of the β phase

In addition, to drive the kinetics, we need:

- M - mobility value for the concentration field
- L - mobility value for the structural order parameter field

3 Variational treatment

From the variational derivatives given in Appendix II, we obtain the chemical potentials for the concentration and the structural order parameters:

$$\mu_c = f_{\alpha,c}\left(1 - H(\eta_1) - H(\eta_2) - H(\eta_3)\right) + f_{\beta,c}\left(H(\eta_1) + H(\eta_2) + H(\eta_3)\right) + \boldsymbol{C}_{ijkl}(-\boldsymbol{\varepsilon}^0_{ij,c})\left(\boldsymbol{\varepsilon}_{kl} - \boldsymbol{\varepsilon}^0_{kl}\right) \tag{8}$$

$$\mu_{\eta_p} = (f_\beta - f_\alpha)H(\eta_p)_{,\eta_p} + W f_{Landau,\eta_p} - \boldsymbol{\kappa}^{\eta_p}_{ij}\eta_{p,ij} + \boldsymbol{C}_{ijkl}(-\boldsymbol{\varepsilon}^0_{ij,\eta_p})\left(\boldsymbol{\varepsilon}_{kl} - \boldsymbol{\varepsilon}^0_{kl}\right) + \frac{1}{2}\boldsymbol{C}_{ijkl,\eta_p}\left(\boldsymbol{\varepsilon}_{ij} - \boldsymbol{\varepsilon}^0_{ij}\right)\left(\boldsymbol{\varepsilon}_{kl} - \boldsymbol{\varepsilon}^0_{kl}\right) \tag{9}$$

4 Kinetics

Now the PDE for Cahn-Hilliard dynamics is given by:

$$\frac{\partial c}{\partial t} = \boldsymbol{\nabla} \cdot (M \boldsymbol{\nabla} \mu_c) \tag{10}$$

and the PDE for Allen-Cahn dynamics is given by:

$$\frac{\partial \eta_p}{\partial t} = -L\mu_{\eta_p} \tag{11}$$

where M and L are the constant mobilities.

5 Mechanics

Considering variations on the displacement u of the from $u + \epsilon w$, we have

$$\delta_u \Pi = \int_\Omega \boldsymbol{\nabla} w : \boldsymbol{C}(\eta_1, \eta_2, \eta_3) : \left(\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^0(c, \eta_1, \eta_2, \eta_3)\right)\, dV = 0 \tag{12}$$

$$\tag{13}$$

where $\boldsymbol{\sigma} = \boldsymbol{C}(\eta_1, \eta_2, \eta_3) : \left(\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^0(c, \eta_1, \eta_2, \eta_3)\right)$ is the stress tensor.

Now consider

$$R = \int_\Omega \boldsymbol{\nabla} w : \boldsymbol{C}(\eta_1, \eta_2, \eta_3) : \left(\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^0(c, \eta_1, \eta_2, \eta_3)\right)\, dV = 0 \tag{14}$$

We solve for $R = 0$ using a gradient scheme which involves the following linearization:

$$R\mid_u + \frac{\partial R}{\partial u}\Delta u = 0 \tag{15}$$

$$\Rightarrow \frac{\partial R}{\partial u}\Delta u = -R\mid_u \tag{16}$$

This is the linear system $Ax = b$ which we solve implicitly using the Conjugate Gradient scheme. For clarity, here in the left hand side (LHS) $A = \frac{\partial R}{\partial u}$, $x = \Delta u$ and the right hand side (RHS) is $b = -R\mid_u$.

6 Time discretization

Using forward Euler explicit time stepping, equations 10 and 11 become:

$$c^{n+1} = c^n + \Delta t[\nabla \cdot (M\nabla\mu_c)] \tag{17}$$

$$\eta_p^{n+1} = \eta_p^n - \Delta t L \mu_{\eta_p} \tag{18}$$

7 Weak formulation

Writing equations 10 and 11 in the weak form, with the arbirary variation given by w yields:

$$\int_\Omega wc^{n+1}dV = \int_\Omega wc^n + w\Delta t[\nabla \cdot (M\nabla\mu_c)]dV \tag{19}$$

$$\int_\Omega w\eta_p^{n+1}dV = \int_\Omega w\eta_p^n - w\Delta t L\mu_{\eta_p}dV \tag{20}$$

The gradient of μ_c is:

$$\begin{aligned}\nabla\mu_c =& \nabla c\left[f_{\alpha,cc} + \sum_{p=1}^{3} H(\eta_p)(f_{\beta,cc} - f_{\alpha,cc})\right] + \sum_{p=1}^{3}\nabla\eta_p H(\eta_p)_{,\eta_p}(f_{\beta,c} - f_{\alpha,c}) \\ &+ \left[\sum_{p=1}^{3}(C_{ijkl}^{\eta_p} - C_{ijkl}^{\alpha})\nabla\eta_p H(\eta_p)_{,\eta_p}\right](-\epsilon_{ij,c}^0)(\epsilon_{ij} - \epsilon_{ij}^0) \\ &- C_{ijkl}\left[\sum_{p=1}^{3} H(\eta_p)_{,\eta_p}\epsilon_{ij,c}^{0\eta_p}\nabla\eta_p + H(\eta_p)\epsilon_{ij,cc}^{0\eta_p}\nabla c\right](\epsilon_{kl} - \epsilon_{kl}^0) \\ &+ C_{ijkl}(-\epsilon_{ij,c}^0)\left[\nabla\epsilon_{ij} - \left(\sum_{p=1}^{3} H(\eta_p)_{,\eta_p}\epsilon_{kl}^{0\eta_p}\nabla\eta_p + H(\eta_p)\epsilon_{kl,c}^{0\eta_p}\nabla c\right)\right]\end{aligned} \tag{21}$$

Applying the divergence theorem to equation 19, one can derive the residual terms r_c and r_{cx}:

$$\int_\Omega wc^{n+1}dV = \int_\Omega w\underbrace{c^n}_{r_c} + \nabla w\cdot(\underbrace{-\Delta t M\nabla\mu_c}_{r_{cx}})dV \tag{22}$$

Expanding μ_{η_p} in equation 20 and applying the divergence theorem yields the residual terms r_{η_p} and $r_{\eta_p x}$:

$$\begin{aligned}&\int_\Omega w\eta_p^{n+1}dV = \\ &\int_\Omega w\Big\{\underbrace{\eta_p^n - \Delta t L\Big[(f_\beta - f_\alpha)H(\eta_p^n)_{,\eta_p} + W f_{Landau,\eta_p} - C_{ijkl}\left(H(\eta_p)_{,\eta_p}\epsilon_{ij}^{0\eta_p}\right)(\epsilon_{kl} - \epsilon_{kl}^0)}_{r_{\eta_p}} \\ &\underbrace{+\frac{1}{2}\left[(C_{ijkl}^{\eta_p} - C_{ijkl}^{\alpha})H(\eta_p)_{,\eta_p}\right](\epsilon_{ij} - \epsilon_{ij}^0)(\epsilon_{kl} - \epsilon_{kl}^0)\Big]\Big\}}_{r_{\eta_p}\ cont.} \\ &+ \nabla w\cdot(\underbrace{-\Delta t L\boldsymbol{\kappa}_{ij}^{\eta_p}\eta_{p,i}^n}_{r_{\eta_p x}})dV\end{aligned} \tag{23}$$

8 Appendix I: Example functions for f_α, f_β, f_{Landau}, $H(\eta_p)$

$$f_\alpha(c) = A_{2,\alpha}c^2 + A_{1,\alpha}c + A_{0,\alpha} \tag{24}$$

$$f_\beta(c) = A_{2,\beta}c^2 + A_{1,\beta}c + A_{0,\beta} \tag{25}$$

$$f_{Landau}(\eta_1,\eta_2,\eta_3) = (\eta_1^2+\eta_2^2+\eta_3^2) - 2(\eta_1^3+\eta_2^3+\eta_3^3) + (\eta_1^4+\eta_2^4+\eta_3^4) + 5(\eta_1^2\eta_2^2+\eta_2^2\eta_3^2+\eta_1^2\eta_3^2) + 5(\eta_1^2\eta_2^2\eta_3^2) \tag{26}$$

$$H(\eta_p) = 3\eta_p^2 - 2\eta_p^3 \tag{27}$$

9 Appendix II: Variational Derivatives

Variational derivative of Π with respect to η_p (where η_q and η_r correspond to the structural order parameters for the other two orientational variants):

$$\delta_{\eta_p}\Pi = \frac{d}{d\alpha}\left[\int_\Omega f_{chem}(c,\eta_p+\alpha w,\eta_q,\eta_r) + f_{grad}(\eta_p+\alpha w,\eta_q,\eta_r) + f_{el}(c,\eta_p+\alpha w,\eta_q,\eta_r,\epsilon)dV\right]_{\alpha=0} \tag{28}$$

Breaking up each of these terms yields:

$$\begin{aligned}
\frac{d}{d\alpha}\left[f_{chem}(c,\eta_p+\alpha w,\eta_q,\eta_r)\right]_{\alpha=0} &= f_\alpha(c)\left[-\frac{\partial H(\eta_p+\alpha w)}{\partial(\eta_p+\alpha w)}\frac{\partial(\eta_p+\alpha w)}{\partial\alpha}\right]_{\alpha=0} \\
&+ f_\beta(c)\left[\frac{\partial H(\eta_p+\alpha w)}{\partial(\eta_p+\alpha w)}\frac{\partial(\eta_p+\alpha w)}{\partial\alpha}\right]_{\alpha=0} \\
&+ W\left[\frac{\partial f_{Landau}(\eta_p+\alpha w,\eta_q,\eta_r)}{\partial(\eta_p+\alpha w)}\frac{\partial(\eta_p+\alpha w)}{\partial\alpha}\right]_{\alpha=0} \\
&= f_\alpha(c)\left[-\frac{\partial H(\eta_p)}{\partial\eta_p}w\right] + f_\beta(c)\left[\frac{\partial H(\eta_p)}{\partial\eta_p}w\right] + W\left[\frac{\partial f_{Landau}(\eta_p,\eta_q,\eta_r)}{\partial\eta_p}w\right]
\end{aligned} \tag{29}$$

$$\begin{aligned}
\frac{d}{d\alpha}\left[f_{grad}(\eta_p+\alpha w,\eta_q,\eta_r)\right]_{\alpha=0} &= \frac{1}{2}\left[\kappa_{ij}^{\eta_p}(\eta_p+\alpha w)_{,i}(\eta_p+\alpha w)_{,j} + \kappa_{ij}^{\eta_q}(\eta_q)_{,i}(\eta_q)_{,j} + \kappa_{ij}^{\eta_r}(\eta_r)_{,i}(\eta_r)_{,j}\right]_{\alpha=0} \\
&= \kappa_{ij}w_{,i}\eta_{p,j}
\end{aligned} \tag{30}$$

$$\begin{aligned}
\frac{d}{d\alpha}\left[f_{el}(c,\eta_p+\alpha w,\eta_q,\eta_r,\epsilon)\right]_{\alpha=0} &= \frac{1}{2}\bigg[\frac{\partial C_{ijkl}(\eta_p+\alpha w,\eta_q,\eta_r)}{\partial(\eta_p+\alpha w)}\frac{\partial(\eta_p+\alpha w)}{\partial\alpha} \\
&\cdot\left(\epsilon_{ij}-\epsilon^0_{ij}(c,\eta_p+\alpha w,\eta_q,\eta_r)\right)\left(\epsilon_{kl}-\epsilon^0_{kl}(c,\eta_p+\alpha w,\eta_q,\eta_r)\right) \\
&+ C_{ijkl}(\eta_p+\alpha w,\eta_q,\eta_r)\left(-\frac{\partial\epsilon^0_{ij}(c,\eta_p+\alpha w,\eta_q,\eta_r)}{\partial(\eta_p+\alpha w)}\frac{\partial(\eta_p+\alpha w)}{\partial\alpha}\right) \\
&\cdot\left(\epsilon_{kl}-\epsilon^0_{kl}(c,\eta_p+\alpha w,\eta_q,\eta_r)\right) \\
&+ C_{ijkl}(\eta_p+\alpha w,\eta_q,\eta_r)\left(\epsilon_{ij}-\epsilon^0_{ij}(c,\eta_p+\alpha w,\eta_q,\eta_r)\right) \\
&\cdot\left(-\frac{\partial\epsilon^0_{kl}(c,\eta_p+\alpha w,\eta_q,\eta_r)}{\partial(\eta_p+\alpha w)}\frac{\partial(\eta_p+\alpha w)}{\partial\alpha}\right)\bigg]_{\alpha=0} \\
&= \frac{1}{2}\left[\frac{\partial C_{ijkl}(\eta_p,\eta_q,\eta_r)}{\partial\eta_p}w\left(\epsilon_{ij}-\epsilon^0_{ij}(c,\eta_p,\eta_q,\eta_r)\right)\left(\epsilon_{kl}-\epsilon^0_{kl}(c,\eta_p,\eta_q,\eta_r)\right)\right] \\
&+ C_{ijkl}(\eta_p,\eta_q,\eta_r)\left(-\frac{\partial\epsilon^0_{ij}(c,\eta_p,\eta_q,\eta_r)}{\partial\eta_p}w\right)\left(\epsilon_{kl}-\epsilon^0_{kl}(c,\eta_p,\eta_q,\eta_r)\right)
\end{aligned} \tag{31}$$

Putting the terms back together yields:

$$
\begin{aligned}
\delta_{\eta_p}\Pi = \int_{\Omega} & f_{\alpha}(c)\left[-\frac{\partial H(\eta_p)}{\partial \eta_p}w\right] + f_{\beta}(c)\left[\frac{\partial H(\eta_p)}{\partial \eta_p}w\right] + W\left[\frac{\partial f_{Landau}(\eta_p,\eta_q,\eta_r)}{\partial \eta_p}w\right] \\
& + \kappa_{ij}w_{,i}\eta_{p,j} \\
& + \frac{1}{2}\left[\frac{\partial C_{ijkl}(\eta_p,\eta_q,\eta_r)}{\partial(\eta_p)}w\big(\epsilon_{ij}-\epsilon^0_{ij}(c,\eta_p,\eta_q,\eta_r)\big)\big(\epsilon_{kl}-\epsilon^0_{kl}(c,\eta_p,\eta_q,\eta_r)\big)\right] \\
& + C_{ijkl}(\eta_p,\eta_q,\eta_r)\left(-\frac{\partial \epsilon^0_{ij}(c,\eta_p,\eta_q,\eta_r)}{\partial \eta_p}w\right)\big(\epsilon_{kl}-\epsilon^0_{kl}(c,\eta_p,\eta_q,\eta_r)\big)\ dV
\end{aligned} \tag{32}
$$

Variational derivative of Π with respect to c :

$$
\delta_c\Pi = \frac{d}{d\alpha}\left[\int_{\Omega} f_{chem}(c+\alpha w,\eta_p,\eta_q,\eta_r) + f_{grad}(\eta_p,\eta_q,\eta_r) + f_{el}(c+\alpha w,\eta_p,\eta_q,\eta_r,\epsilon)dV\right]_{\alpha=0} \tag{33}
$$

Breaking up each of these terms yields:

$$
\begin{aligned}
\frac{d}{d\alpha}\left[f_{chem}(c+\alpha w,\eta_p,\eta_q,\eta_r)\right]_{\alpha=0} &= \Bigg[\frac{\partial f_{\alpha}(c+\alpha w)}{\partial(c+\alpha w)}\frac{\partial(c+\alpha w)}{\partial \alpha}\left(1-\sum_{p=1}^{3}H(\eta_p)\right) \\
&\quad + \frac{\partial f_{\beta}(c+\alpha w)}{\partial(c+\alpha w)}\frac{\partial(c+\alpha w)}{\partial \alpha}\left(\sum_{p=1}^{3}H(\eta_p)\right) + W\frac{\partial f_{Landau}(\eta_p,\eta_q,\eta_r)}{\partial(c+\alpha w)}\frac{\partial(c+\alpha w)}{\partial \alpha}\Bigg]_{\alpha=0} \\
&= \frac{\partial f_{\alpha}(c)}{\partial c}w\left(1-\sum_{p=1}^{3}H(\eta_p)\right) + \frac{\partial f_{\beta}(c)}{\partial c}w\left(\sum_{p=1}^{3}H(\eta_p)\right)
\end{aligned} \tag{34}
$$

$$
\frac{d}{d\alpha}\left[f_{grad}(\eta_p,\eta_q,\eta_r)\right]_{\alpha=0} = 0 \tag{35}
$$

$$
\begin{aligned}
\frac{d}{d\alpha}\left[f_{el}(c+\alpha w,\eta_p,\eta_q,\eta_r,\epsilon)\right]_{\alpha=0} &= \frac{1}{2}C_{ijkl}(\eta_p,\eta_q,\eta_r)\Bigg[-\frac{\partial \epsilon^0_{ij}(c+\alpha w,\eta_p,\eta_q,\eta_r)}{\partial(c+\alpha w)}\frac{\partial(c+\alpha w)}{\partial \alpha}\big(\epsilon_{kl}-\epsilon^0_{kl}(c+\alpha w,\eta_p,\eta_q,\eta_r)\big) \\
&\quad - \big(\epsilon_{ij}-\epsilon^0_{ij}(c+\alpha w,\eta_p,\eta_q,\eta_r)\big)\frac{\partial \epsilon^0_{ij}(c+\alpha w,\eta_p,\eta_q,\eta_r)}{\partial(c+\alpha w)}\frac{\partial(c+\alpha w)}{\partial \alpha}\Bigg]_{\alpha=0} \\
&= -C_{ijkl}(\eta_p,\eta_q,\eta_r)\frac{\partial \epsilon^0_{ij}(c,\eta_p,\eta_q,\eta_r)}{\partial c}w\big(\epsilon_{kl}-\epsilon^0_{kl}(c+\alpha w,\eta_p,\eta_q,\eta_r)\big)
\end{aligned} \tag{36}
$$

Putting the terms back together yields:

$$
\begin{aligned}
\delta_c\Pi = \int_{\Omega} & \frac{\partial f_{\alpha}(c)}{\partial c}w\left(1-\sum_{p=1}^{3}H(\eta_p)\right) + \frac{\partial f_{\beta}(c)}{\partial c}w\left(\sum_{p=1}^{3}H(\eta_p)\right) \\
& - C_{ijkl}(\eta_p,\eta_q,\eta_r)\frac{\partial \epsilon^0_{ij}(c,\eta_p,\eta_q,\eta_r)}{\partial c}w\big(\epsilon_{kl}-\epsilon^0_{kl}(c+\alpha w,\eta_p,\eta_q,\eta_r)\big)\ dV
\end{aligned} \tag{37}
$$